
Applications of Lie group integrators and exponential schemes

*Workshop on Lie group methods and control
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Brynjulf Owren

Dept of Math Sci, NTNU



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Outline

PART I (Introductory)

- Linear IVPs, Eigenvalue problems, linear PDEs
- Manifolds (“stay on manifold” principle)
- Classical problems (“curved path” principle)

PART II (Recent results on exp ints)

- A unified approach to exponential integrators
- Order theory
- Bounds for dimensions of involved function spaces



I.1 Linear IVPs

One may for instance write

$$\dot{\mathbf{u}} = \mathbf{A}(t) \mathbf{u}, \quad \mathbf{A} : \mathbb{R} \rightarrow \mathbb{R}^{n \times n}$$

In literature, usually $\mathbf{u} \in \mathbb{R}^n$.

LGI: Magnus series or related (Cayley etc)

When/Why use this scheme.

1. Highly oscillatory ODEs, large imaginary eigenvalues.
Iserles
2. PDEs, $\mathbf{A}(t)$ unbounded, classical example: Linear Schrödinger equation (LSE)). Blanes & Moan, Hochbruck & Lubich.
Recently also Landau-Lifschitz equation Sun, Qin, Ma



I.1 Magnus works on LSE!

$i \frac{du}{dt} = H(t) u$, $H(t)$ unbounded, selfadjoint

$d \exp_u$ is not invertible for $2k\pi i \in \sigma(u)$, $k \in \mathbb{Z} \setminus \{0\}$.

Truncated series is still unbounded at ∞ .

H & L find error bounds of the form

$$\|u_m - u(t_m)\| = C h^p t_m \max_{0 \leq t \leq t_m} \|D^{p-1} u(t)\|$$

D is a “differentiation operator” related to the LSE.



Eigenvalue problems

Stability of travelling wave solutions to PDEs. Boils down to eigenvalue problem

$$\dot{\mathbf{Y}} = A(t, \lambda) \mathbf{Y}$$

where λ is a parameter.

Needs to be solved for several λ .

Magnus integrators used with success by Malham, Oliver and others.

Early work by Moan on such problems.



I.2 Problems on (nonlinear) manifolds

A large part of the applications I know involves the **orthogonal group** which acts transitively on either of

- The orthogonal group itself (or its tangent bundle).
- Stiefel manifold. ($n \times p$ matrices with orthonormal columns)
- The $n - 1$ -sphere. (Stiefel with $p = 1$)



I.2 Orthogonal group problems

Most used examples are on $n = 3$ (3D rotations): Free rigid body, spinning top, . . .

Scheme. Most LGIs work. RKMK, Crouch-Grossmann, . . . combined with all possible “coordinates” exp, Cayley, CCSK etc.

My evaluation

- Most Lie group integrators do little else for you than maintaining orthogonality.
- Poor long-time behaviour.
- Hard to get reversible / symplectic schemes.
- There are exceptions (Lewis and Simo, Zanna et al.) but these LGIs seem expensive.



I.2 Stiefel manifolds

Some applications which involve computation on Stiefel manifolds

- Computation of Lyapunov exponents
- Multivariate data analysis (optimisation, gradient flows)
- Neural networks, Independent Component Analysis

Demands. Maintain orthonormality. Inexpensive stepping, cost $\mathcal{O}(np^2)$ per step.

Schemes. Most LGIs work. RKM_K, Crouch-Grossmann, ... combined with all possible “coordinates” exp, Cayley, CCSK etc. Most of them can be implemented in $\mathcal{O}(np^2)$ ops per step, but special care must be taken.



I.2 Stiefel manifolds

My evaluation

- Lie group integrators meet requirements specified in literature
- Long-time behaviour has not been an issue.
- Overall judgement: Lie group integrators are competitive, if not superior to classical integrators.

Sources

- Dieci, Van Vleck [schemes, but also general viewpoints, Lyapunov exponents]
- Trendafilov. [Multivariate data analysis]
- Celledoni, Fiori.[Neural nets, ICA]
- LGIs for Stiefel, Krogstad, Celledoni + O

I.2 Other manifold applications

- Certain PDEs whose solution evolve on (copies of) S^{n-1} , Lie group integrators have been used.
- Some special types of manifolds, e.g described by quadratic invariants like oblique manifold, DelBuono, Lopez.



I.2 Conclusions

- There are several manifold applications where Lie group integrators now represent an alternative choice. Recent research have caused implementations to be much less expensive.
- Their best feature is that they preserve the manifold. I have seen little evidence to suggest that Lie group integrators is natural for maintaining additional geometric structure. Is there hope for improvement on this point?
- The development of Lie group integrators has added important insight in the integration of DEs on manifolds. Understanding of numerics has become less dependent on specific **coordinates** and **embeddings**.



I.2 Conclusions (2)

The activity on Lie group integrators has caused progress in fields related to geometric integration:

- Computing the matrix exponential
- Computing highly oscillatory integrals
- Analysis of split-step schemes
- Exponential integrators
- Algebraic structure on trees, Hopf algebras
- Computation with the BCH-formula



I.3 Curved path principle

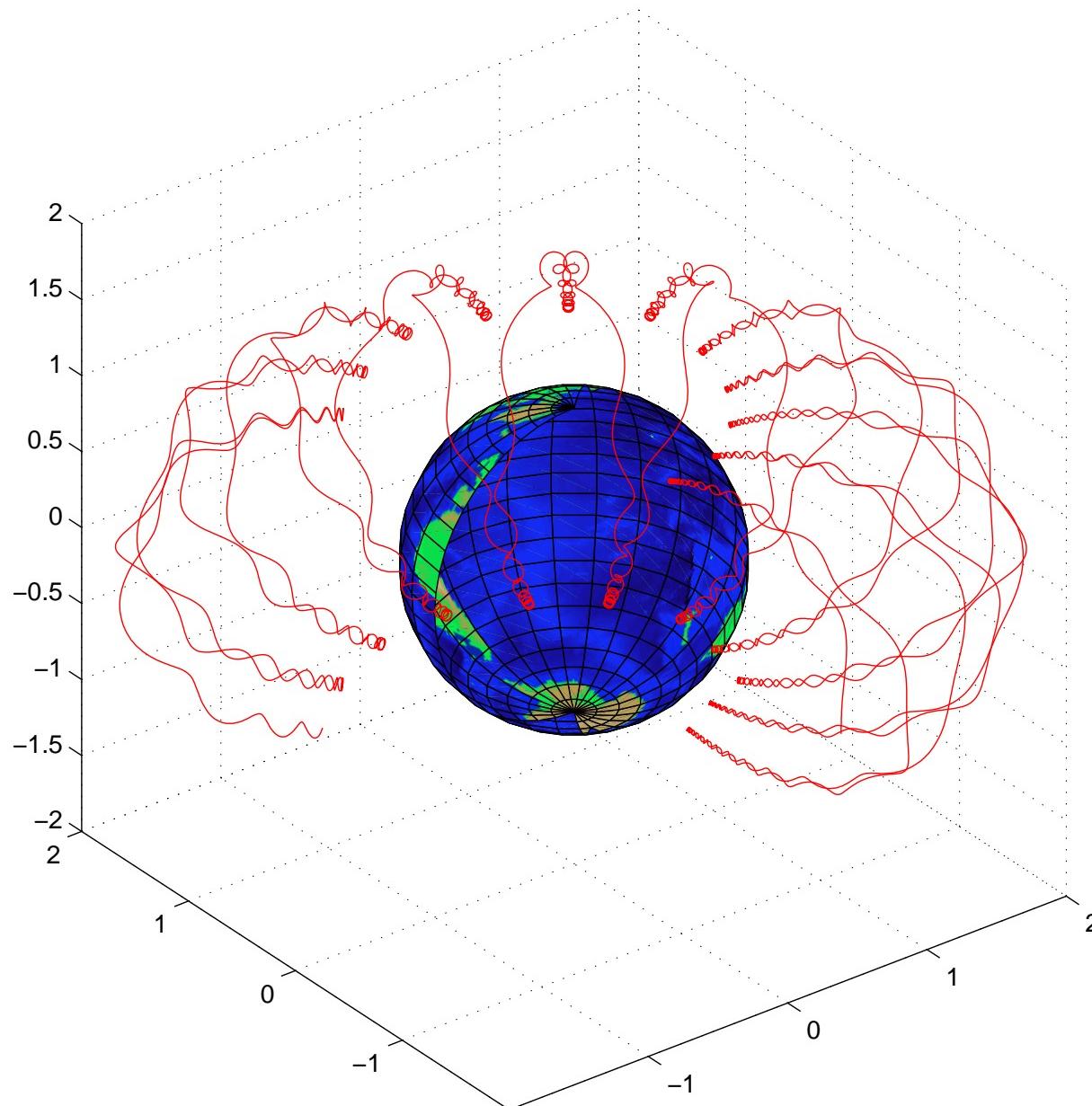
- Classical numerical ODE-solvers progress solution along straight lines.
- Lie group integrators map a straight line in some other space (Lie algebra) to phase space through a nonlinear map.
- Allows for much more general “movements”.

Two excellent examples provided by [Munthe-Kaas](#).

1. The [northern light](#) equations.
2. PDEs with perturbation terms by [affine action](#)



I.3 Northern light



I.3, II Time Integrators for Nonlinear PDEs

Many PDEs are of the (abstract) form

$$\mathbf{u}_t = \mathbf{L} \mathbf{u} + \mathbf{N}(\mathbf{u})$$

\mathbf{L} : unbounded linear operator (like Δ)

$\mathbf{N}(\mathbf{u})$: a (relatively) small nonlinear term.

Includes: NLS, Nonlinear heat equations, KdV, Allen–Cahn, Kuramoto–Sivashinsky, and many more.

Unbounded \mathbf{L} requires a form of implicit integrator.

One wants an explicit scheme for the nonlinear part.

Many time integrators are known for this purpose.



Main Classes of Time Integrators

- LI** Linearly implicit or **IMEX** methods ([Varah](#), [Ruuth](#), [Ascher](#), [Russo](#) and many more)
- SS** Split step methods ([Godunov](#), [Strang](#) etc)
- IF** Integrating factor methods ([Lawson](#), [Nørsett](#))
- SL** Sliders ([Fornberg](#), [Driscoll](#))
- ETD** Exponential Time Differencing ([Cox](#), [Matthews](#), now also [Krogstad](#))
- LGI** Lie group integrators with special actions ([Munthe-Kaas](#) and others).



Exact or Rational

Among all these schemes, some use **exact partial flows**, others use **rational approximants** for the unbounded part.

Claim

Real eigenvalues of $\textcolor{red}{L}$ favour **rational approxmants**,
imaginary eigenvalues favour **exact partial flows**.

Henceforth we consider only schemes which apply **exact partial flows** (ie. “exact up to space discretization”)



Assumptions

In what follows, we shall always assume

- Whenever $\mathbf{L} = \mathbf{0}$ the scheme reduces to a classical RK scheme for the problem $\mathbf{u}_t = \mathbf{N}(\mathbf{u})$
- Whenever $\mathbf{N}(\mathbf{u}) \equiv \mathbf{0}$, the exact solution of $\mathbf{u}_t = \mathbf{L}\mathbf{u}$ is recovered.

The classical Runge-Kutta scheme obtained when $\mathbf{L} = \mathbf{0}$ is denoted “The underlying RK-scheme”

Our favourite choice for underlying RK scheme is the classical RK4.

Classical Runge-Kutta 4 (RK4C)

Problem of form $u_t = N(u)$. Step from t_0 to $t_0 + h$

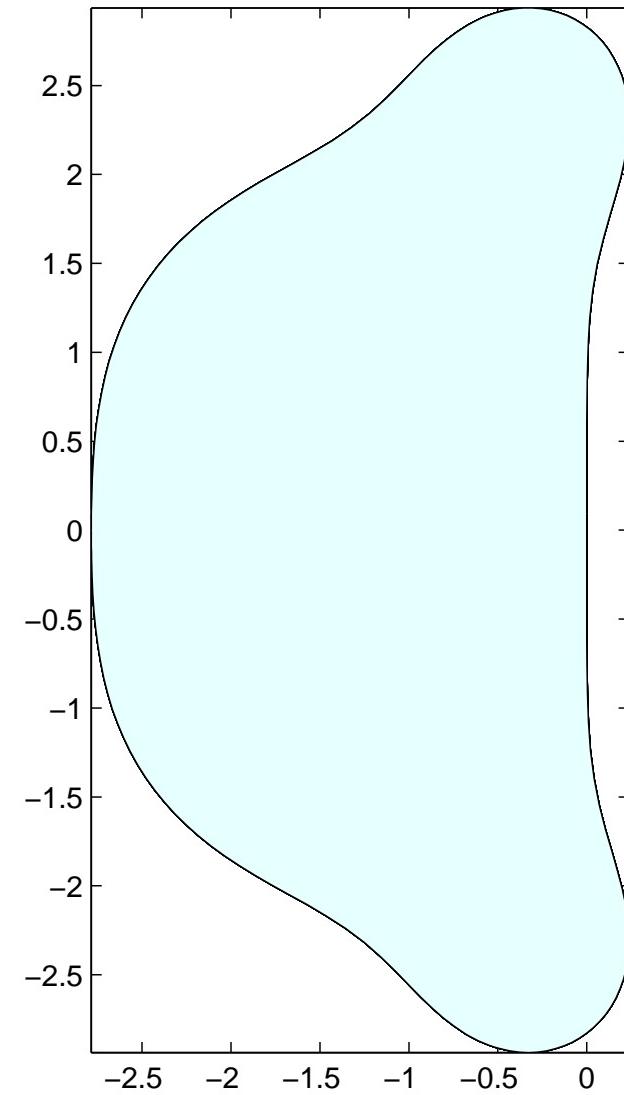
$$N_1 = N(u_0)$$

$$N_2 = N(u_0 + \frac{1}{2}hN_1)$$

$$N_3 = N(u_0 + \frac{1}{2}hN_2)$$

$$N_4 = N(u_0 + hN_3)$$

$$u_1 = u_0 + \frac{h}{6}(N_1 + 2N_2 + 2N_3 + N_4)$$



An Integrating Factor Scheme (LAW4)

Lawson (1967) derived the schemes by setting

$$v(t) = \exp(-tL)u(t)$$

which leads to $v_t = \tilde{N}(v)$ where $\tilde{N} = e^{tL} \circ N \circ e^{-tL}$.
Solve resulting equation by RK4C.

$$\mathbf{N}_1 = N(u_0)$$

$$\mathbf{N}_2 = N(e^{\frac{h}{2}L}(u_0 + \frac{1}{2}h\mathbf{N}_1))$$

$$\mathbf{N}_3 = N(e^{\frac{h}{2}L}u_0 + \frac{1}{2}h\mathbf{N}_2)$$

$$\mathbf{N}_4 = N(e^{hL}u_0 + e^{\frac{h}{2}L}h\mathbf{N}_3)$$

$$u_1 = e^{hL}u_0 + \frac{h}{6}(e^{hL}\mathbf{N}_1 + 2e^{\frac{h}{2}L}(\mathbf{N}_2 + \mathbf{N}_3) + \mathbf{N}_4)$$



Lie Group Methods and the Affine Action

The scheme is based on the **affine Lie group action**.

Discrete case: Let G be a matrix group over \mathbb{C} with Lie algebra \mathfrak{g} . Pairs $(M, b) \in G \times \mathbb{C}^N$ act on points in \mathbb{C}^N

$$(M, b) \cdot x = Mx + b$$

The Lie algebra consists of pairs $(A, b) \in \mathfrak{g} \times \mathbb{C}^N$.

Exponential map

$$\text{Exp}(t(A, b)) = (e^{tA}, \frac{e^{tA} - 1}{A} b).$$

Commutator

$$[(A_1, b_1), (A_2, b_2)] = [A_1 A_2 - A_2 A_1, A_1 b_2 - A_2 b_1].$$

Here, set $\mathfrak{g} = \text{span}\{L\}$.



An RK–Munthe-Kaas Scheme (RKMK4)

From Munthe-Kaas & Owren (1999) we derive

$$\mathbf{N}_1 = \mathbf{N}(u_0)$$

$$\mathbf{N}_2 = \mathbf{N}\left(e^{\frac{hL}{2}}u_0 + \frac{h}{2}\phi_0\left(\frac{hL}{2}\right)\mathbf{N}_1\right)$$

$$\mathbf{C}_1 = hL(\mathbf{N}_2 - \mathbf{N}_1)$$

$$\mathbf{N}_3 = \mathbf{N}\left(e^{\frac{hL}{2}}u_0 + \phi_0\left(\frac{hL}{2}\right)\left(\frac{h}{2}\mathbf{N}_2 - \frac{h}{8}\mathbf{C}_1\right)\right)$$

$$\mathbf{N}_4 = \mathbf{N}\left(e^{hL}u_0 + \phi_0(hL)h\mathbf{N}_3\right)$$

$$\mathbf{C}_2 = hL(\mathbf{N}_1 - 2\mathbf{N}_2 + \mathbf{N}_4)$$

$$u_1 = e^{hL}u_0 + \frac{h}{6}\phi_0(hL)(\mathbf{N}_1 + 2\mathbf{N}_2 + 2\mathbf{N}_3 + \mathbf{N}_4 - \mathbf{C}_1 - \frac{1}{2}\mathbf{C}_2)$$

where $\phi_0(z) = \frac{e^z - 1}{z}$



A Commutator-Free Lie Group Integrator, Cf4

Celledoni et al. (2002)

$$\mathbf{N}_1 = \mathbf{N}(\mathbf{u}_0)$$

$$\mathbf{U}_2 = e^{\frac{hL}{2}} \mathbf{u}_0 + \frac{h}{2} \phi_0\left(\frac{hL}{2}\right) \mathbf{N}_1$$

$$\mathbf{N}_2 = \mathbf{N}(\mathbf{U}_2)$$

$$\mathbf{N}_3 = \mathbf{N}\left(e^{\frac{hL}{2}} \mathbf{u}_0 + \frac{h}{2} \phi_0\left(\frac{hL}{2}\right) \mathbf{N}_2\right)$$

$$\mathbf{N}_4 = \mathbf{N}\left(e^{\frac{hL}{2}} \mathbf{U}_2 + h \phi_0\left(\frac{hL}{2}\right) \left(\mathbf{N}_3 - \frac{1}{2} \mathbf{N}_1\right)\right)$$

$$\mathbf{U}_s = e^{\frac{hL}{2}} \mathbf{u}_0 + \frac{h}{12} \phi_0\left(\frac{hL}{2}\right) (3\mathbf{N}_1 + 2\mathbf{N}_2 + 2\mathbf{N}_3 - \mathbf{N}_4)$$

$$\mathbf{u}_1 = e^{\frac{hL}{2}} \mathbf{U}_s + \frac{h}{12} \phi_0\left(\frac{hA}{2}\right) (-\mathbf{N}_1 + 2\mathbf{N}_2 + 2\mathbf{N}_3 + 3\mathbf{N}_4)$$



A Cox and Matthews Scheme (C-M4)

This scheme has the same $\mathbf{N}_1, \dots, \mathbf{N}_4$ as Cf4.

$$u_1 = e^{hA} u_0 + h(f_2(hL)\mathbf{N}_1 + 2f_3(hL)(\mathbf{N}_2 + \mathbf{N}_3) + f_4(hL)\mathbf{N}_4)$$

where

$$f_2(z) = \frac{-4 - z + e^z(4 - 3z + z^2)}{z^3}$$

$$f_3(z) = \frac{2 + z + e^z(-2 + z)}{z^3}$$

$$f_4(z) = \frac{-4 - 3z - z^2 + e^z(4 - z)}{z^3}$$

Derivation technique: Unknown!

A unified format

By carefully studying all these schemes, one finds that they all fit into the framework

$$N_r = N(e^{c_r hL} u_0 + h \sum_{j=1}^s a_r^j(hL) N_j), \quad r = 1, \dots, s$$

$$u_1 = e^{hL} u_0 + h \sum_{r=1}^s b^r(hL) N_r.$$

$$a_r^j(z) = \sum_m \alpha_r^{j,m} z^m, \quad b^r(z) = \sum_m \beta^{r,m} z^m$$

$(\alpha_r^{j,0}), (\beta^{r,0})$ underlying RK scheme.

Order theory

Order conditions and $\textcolor{red}{B}$ -series can be derived by standard tools (rooted trees).

$\textcolor{red}{T}$: The set of bicolored rooted trees where each white node has at most 1 child.

$\textcolor{red}{T}'$: Subset of $\textcolor{red}{T}$ where each white node has precisely one child (no white leaves)

$$W_+ : \tau \mapsto \begin{array}{c} \textcolor{red}{\tau} \\ \textcolor{white}{\circ} \end{array}, \quad B_+ : \{\tau_1, \dots, \tau_m\} \mapsto \begin{array}{c} \tau_1 \ \tau_2 \cdot \tau_m \\ \backslash \quad \backslash \quad \backslash \\ \bullet \end{array}$$

- $\textcolor{red}{B}$ -series indexed by $\textcolor{red}{T}$.
- Order conditions: $\textcolor{red}{T}'$ suffices.

Order conditions for exponential integrators

An exponential integrator has order p if

$$u_1(\tau) = \frac{1}{\gamma(\tau)}, \quad \text{for all } \tau \in T' \text{ such that } |\tau| \leq p,$$

where

$$u_1(\emptyset) = U_r(\emptyset) = 1, \quad 1 \leq r \leq s,$$

$$u_1(W_+^m B_+(\tau_1, \dots, \tau_\mu)) = \sum_r \beta^{r,m} U_r(\tau_1) \cdots U_r(\tau_\mu)$$

$$U_r(W_+^m B_+(\tau_1, \dots, \tau_\mu)) = \sum_j \alpha_r^{j,m} U_j(\tau_1) \cdots U_j(\tau_\mu)$$



Number of conditions

Generating function for $\#$ trees with q nodes in T'

$$M(x) = \frac{x}{1-x} \exp \left(M(x) + \frac{M(x^2)}{2} + \frac{M(x^3)}{3} + \dots \right)$$

The number of order conditions for each order **1** to **9** is
1, 2, 5, 13, 37, 108, 332, 1042, 3360.

Coefficient function spaces

$a_r^j(z)$, $b^r(z)$ belong to some function spaces we denote V_a , V_b of finite dimension.

Often, V_a , V_b they are related to the functions

$$\phi_k(z) = \int_0^1 e^{(1-\theta)z} \theta^k d\theta, \quad \text{e.g. } \phi_0(z) = \frac{e^z - 1}{z}$$

Scheme	V_a	V_b
Cf4	$\phi_0(\frac{z}{2}), z\phi_0(\frac{z}{2})^2$	$\phi_0(\frac{z}{2}), \phi_0(z)$
C-M4	As Cf4	$\phi_0(z), \phi_1(z), \phi_2(z)$
RKMK4:	$\phi_0(\frac{z}{2}), z\phi_0(\frac{z}{2})$	$\phi_0(z), z\phi_0(z)$
Law4:	$1, e^{z/2}$	$1, e^{z/2}, e^z$

Assumption and bounds

Let \mathbf{V} of $\dim \mathbf{K}$ be a function space as above.

Assumption. The map

$$f \in \mathbf{V} \mapsto (f(0), f'(0), \dots, f^{(K-1)}(0)) \in \mathbf{R}^K$$

is injective

Theorem. For any p th order exponential integrator, one has

$$K_a = \dim V_a \geq \left\lfloor \frac{p}{2} \right\rfloor, \quad K_b = \dim V_b \geq \left\lfloor \frac{p+1}{2} \right\rfloor.$$

Moreover, the lower bound for V_b is always attainable with basis $\phi_0, \dots, \phi_{K_b-1}$

Remarks

- We have no general proof that lower bound for K_a is sharp. However, with $p = 5$ one can use $K_b = 2$ with $\phi_1(z), \phi_1(\frac{3}{5}z)$.
- A procedure for constructing exponential integrators has been developed. One starts with an arbitrary underlying scheme as well as V_a, V_b .
- The really interesting part is still ahead: Choose spaces V_a, V_b to deal with unbounded L . In the time to come, we focus in particular on the NLS.



Natural Continuous Extensions Zennaro 1986

Let $(\alpha_r^{j,0})$ ($\beta_r^{r,0}$) define an underlying Runge-Kutta scheme of order p

Suppose that polynomials $w_1(\theta), \dots, w_s(\theta)$ of degree d can be found such that

$$\bar{N}(t_0 + \theta h) := \sum_r w'_r(\theta) N_r$$

satisfies

$$\max_{t_0 \leq t \leq t_1} |N(u(t)) - \bar{N}(t)| = \mathcal{O}(h^{d-1})$$

$$\int_{t_0}^{t_1} G(t)(N(u(t)) - \bar{N}(t)) dt = \mathcal{O}(h^{p+1})$$

NB! Requires $a_r^j(z)$ to be given.



NCEs continued

Replace $\mathbf{u}_t = \mathbf{L} \mathbf{u} + \mathbf{N}(\mathbf{u})$ by $\mathbf{v}_t = \mathbf{L} \mathbf{v} + \bar{\mathbf{N}}(t)$, solve exactly, and set $\mathbf{u}_1 := \mathbf{v}(h)$. Yields exponential integrator of order \mathbf{p} with

$$\begin{aligned} b^r(z) &= \int_0^1 \exp((1-\theta)z) w'_r(\theta) d\theta \\ &= \beta^{r,0} + z \int_0^1 \exp((1-\theta)z) w_r(\theta) d\theta \end{aligned}$$

In particular, these are expressed in terms of

$$\phi_k(z) = \int_0^1 \exp(z(1-\theta)) \theta^k d\theta, \quad k = 0, 1, \dots$$

We have rediscovered the Cox& Matthews schemes.

Why it works

$$(u - v)_t = L(u - v) + (N(u) - \bar{N}(t))$$



$$\begin{aligned} (u - v)(t_1) &= \int_{t_0}^{t_1} e^{(t_1-t)L} (N(u(t) - \bar{N}(t)) dt \\ &= \mathcal{O}(h^{p+1}) \end{aligned}$$

thanks to the definition of NCEs

Theorem of Zennaro

The following result gives us a sharp lower bound for the number of ϕ_k functions which must be included

Any NCE satisfies

$$q := \left[\frac{p+1}{2} \right] \leq d \leq \min\{p, s^*\}.$$

Moreover, and NCE of degree q always exists.

Conclusion. An underlying RK scheme of order p can always be extended to an exponential integrator of order p where

$$b^r(z) \in \text{span}\{\phi_0, \dots, \phi_{q-1}\}, \forall r$$

The nonlinear Schrödinger equation

Generally

$$iu_t = -\Delta u + (V(x) + \lambda |u|^{2\sigma}) u, \quad (t, x) \in \mathbb{R} \times \mathbb{R}^d$$

Here

$$0 < \sigma, \quad \text{and} \quad \sigma < \frac{2}{d-2} \quad \text{if} \quad d \geq 3.$$

- Potential: $V(x) \in L_1 + L_\infty$.
- IC: $u(x, 0) = u_0 \in \Sigma \subset H^1$.
- Here, let $d = 1$ and $(x, t) \in S^1 \times \mathbf{R}$.
- Usually, take $\sigma = 1$ (cubic case).



Spectral Discretisation in Space

Use $2n$ modes and set

$$c^k(t) = \sum_{m=-n}^{n-1} U\left(\frac{2m\pi}{2n}, t\right) e^{-imk}$$

leading to the NLS spectrally discretised system

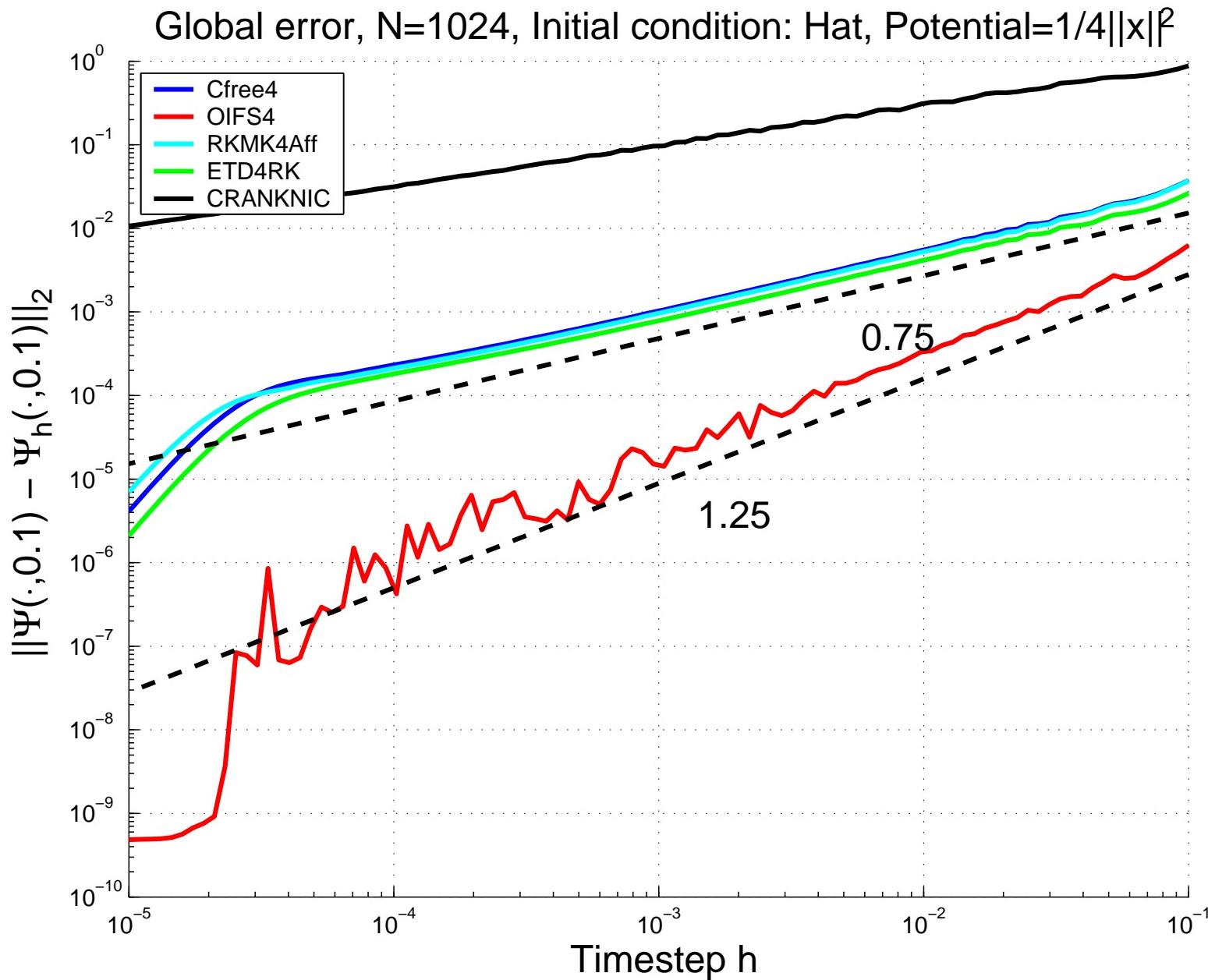
$$\frac{dc}{dt} = D c + \mathcal{F}_n \circ \check{N} \circ \mathcal{F}_n^{-1}(c)$$

$$D = \text{diag}(-ik^2)_{k=-n}^{n-1}$$

$$i\check{N}(U)_\ell = (V(x_\ell) + \lambda|U(x_\ell)|^2)U(x_\ell).$$



NumExp 1



A Simplified Case

Let us

- Focus on one scheme, say the Cf4 scheme.
- For analysis, set $V(x) \equiv v$ and $\lambda = 0$.

In this case, the SDNLS decouples into scalar equations

$$\dot{c}^k = \alpha_k c^k + \beta^k$$

where $\alpha_k = -ik^2$, and $\beta = -iv$.

Setting $a_k = \frac{\beta}{\alpha_k}$, $m_k = e^{-\frac{i}{2}hk^2}$ the Cf4 scheme is

$$c_1 = p(m_k, a_k)c_0, \quad p(m, a) = \sum_{j=0}^5 r_j(a)m^j, \quad r_j \in \Pi_4[a]$$

Global Error Cf4

Need to find global error at $t = T$.

Must estimate $|p_k^n - e_k^n|$ where $n = T/h$

$$p_k = p(m_k, a_k), \quad e_k = \exp(-ih(k^2 + v))$$

A rigorous analysis shows that up to leading order

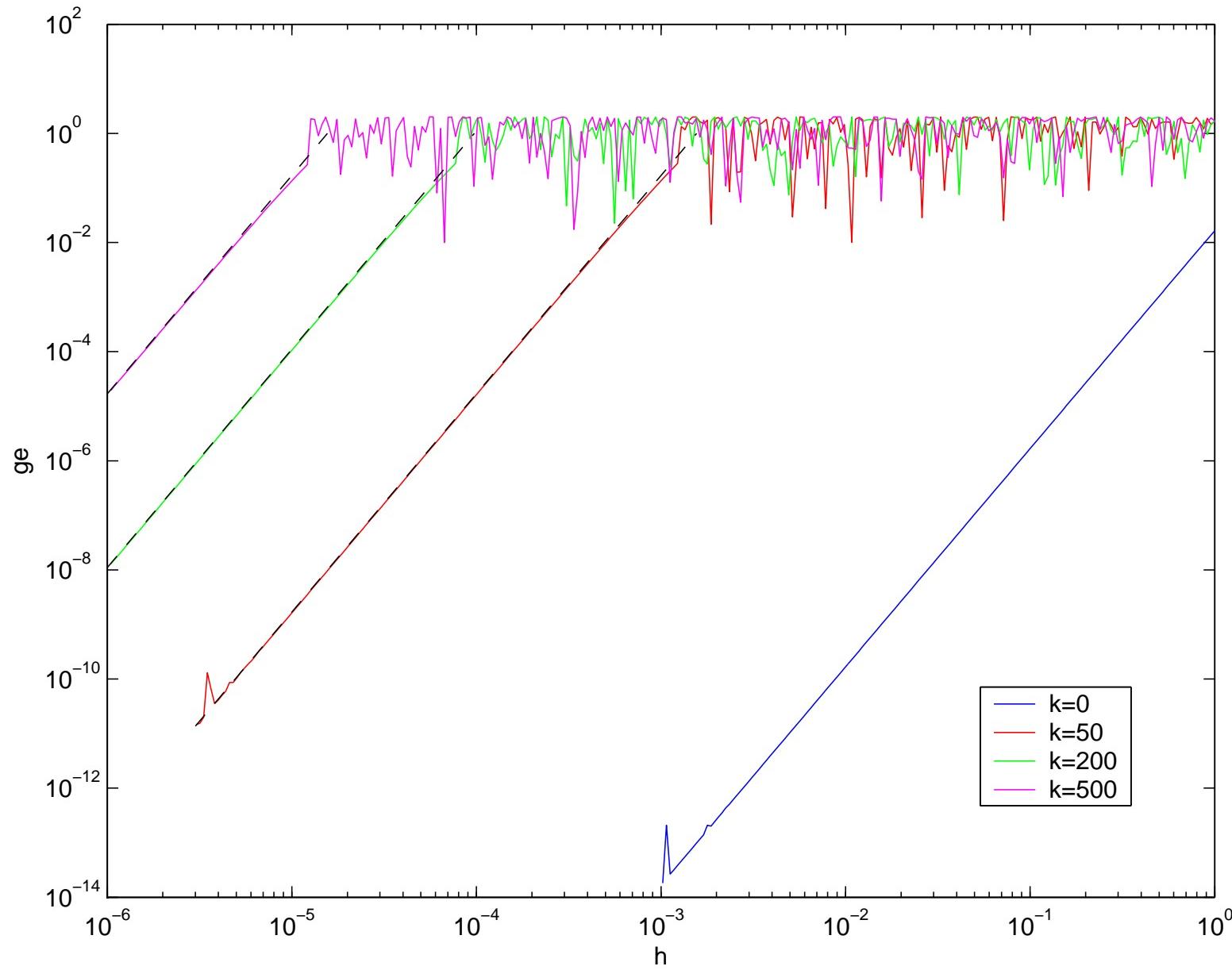
$$|p_k^n - e_k^n| \approx \left(\frac{hk^2}{S_b} \right)^4, \quad S_b = \left(\frac{480}{T|v|} \right)^4$$

whenever $hk^2 \ll 1$ whereas for $hk^2 \gg 1$ (and $|v| \leq \frac{1}{2}k^2$)

$$|p_k^n - e_k^n| \leq 2$$



The Global Error for Decoupled Case



Summing It Up

The ℓ_2 -norm of the global error is found by summing up

$$\|\text{ge}\|^2 = \sum_k |p_k^n - e_k^n|^2 |c_0^k|^2.$$

We may assume that $|c_0^k| \leq \frac{K_0}{k^p}$ (holds in particular if u_0 is $C^p(S^1, \mathbb{C})$). Assuming that $N^2 h \gg 1$ we estimate by Euler–Maclaurin's formula

$$\|\text{ge}\| \approx C h^{\frac{2p-1}{4}}, \quad p \leq 8.$$

Figure 1

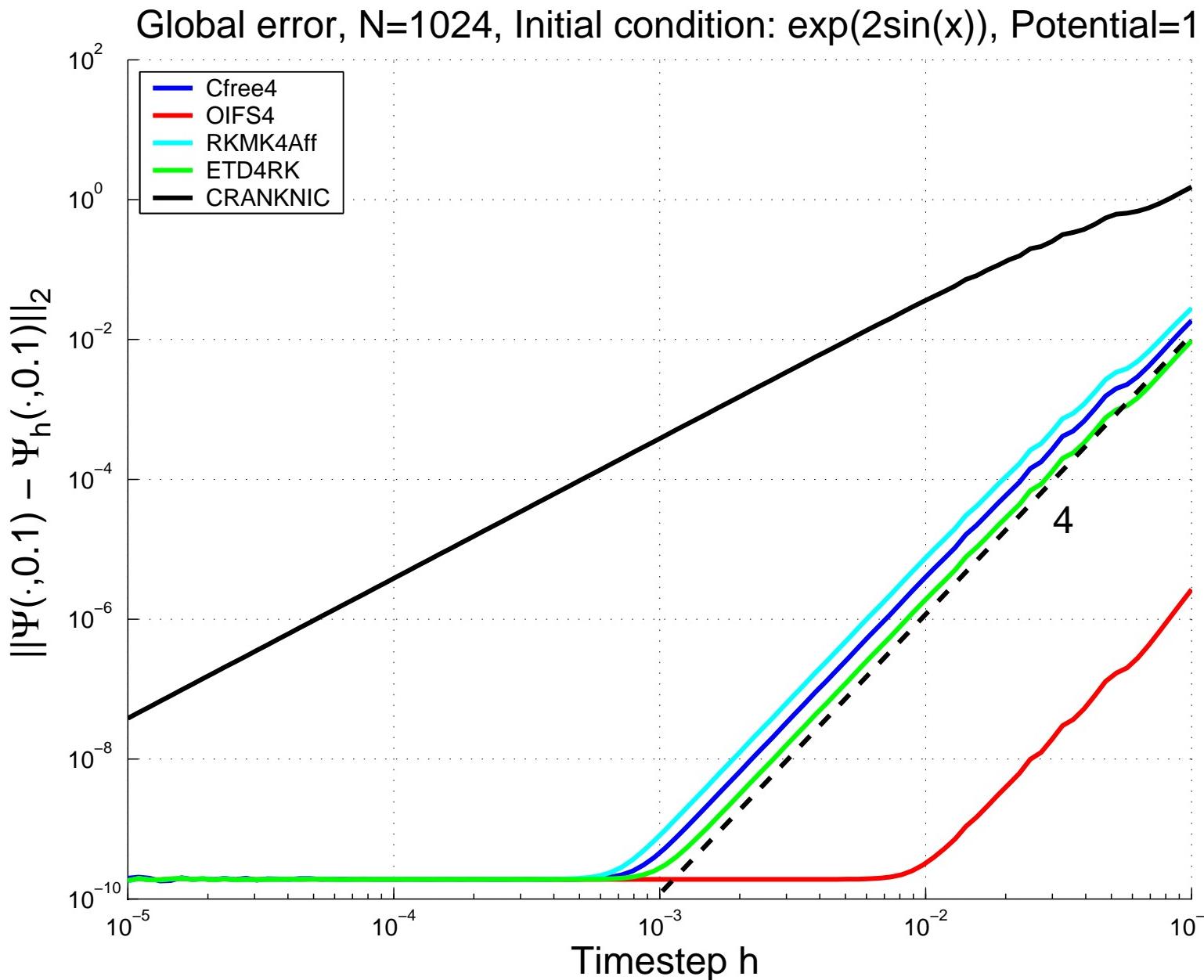


Figure 2

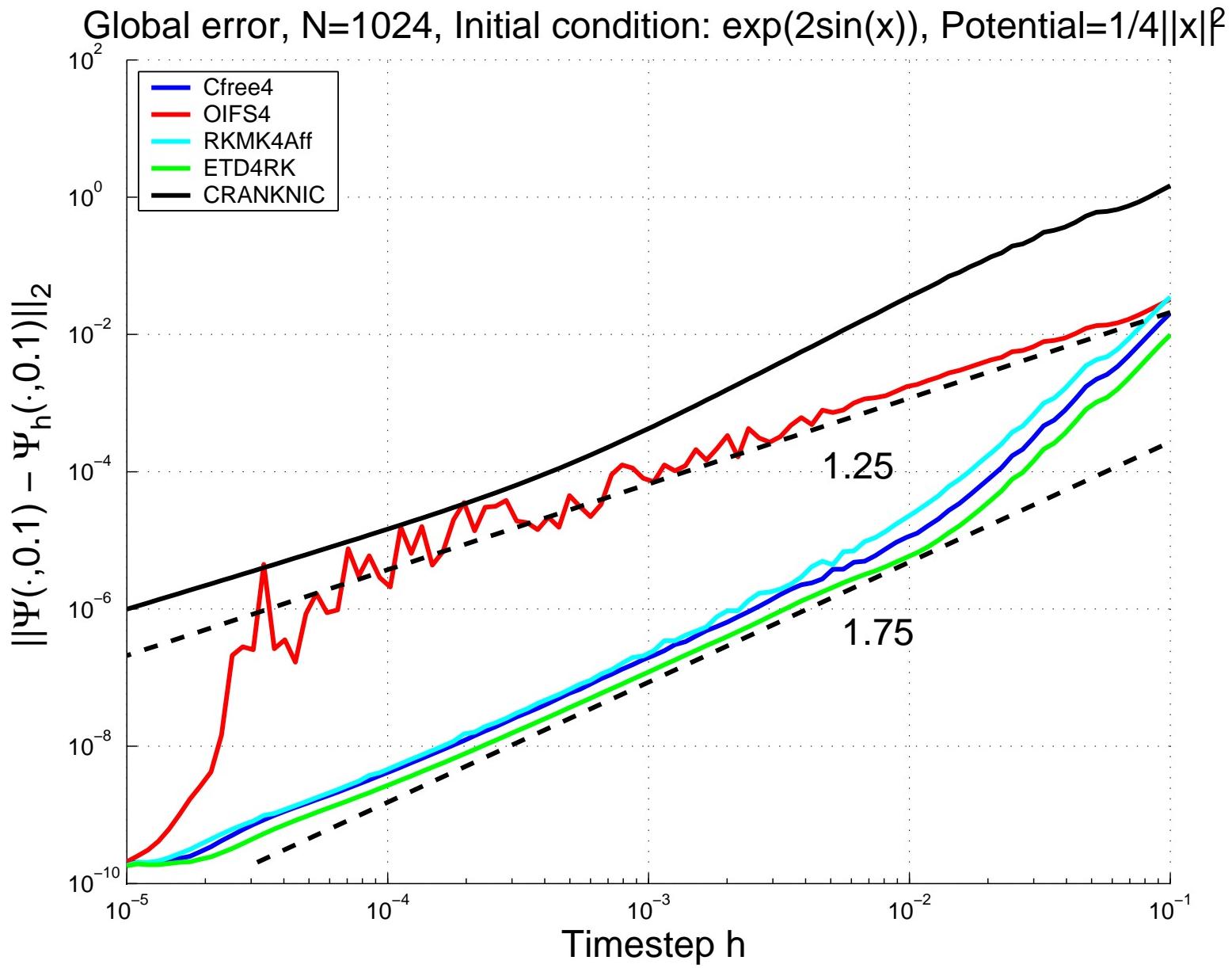


Figure 3

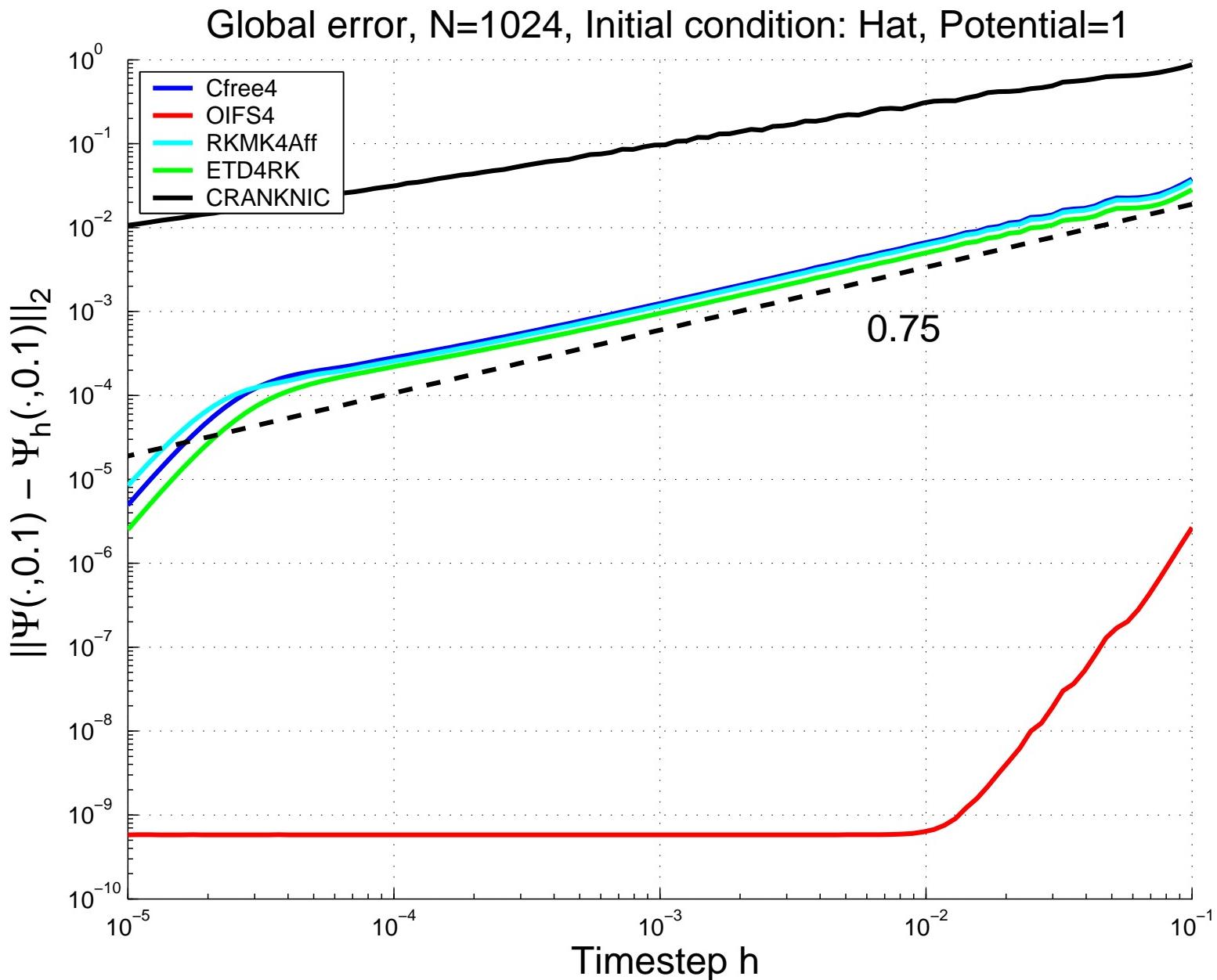


Figure 4

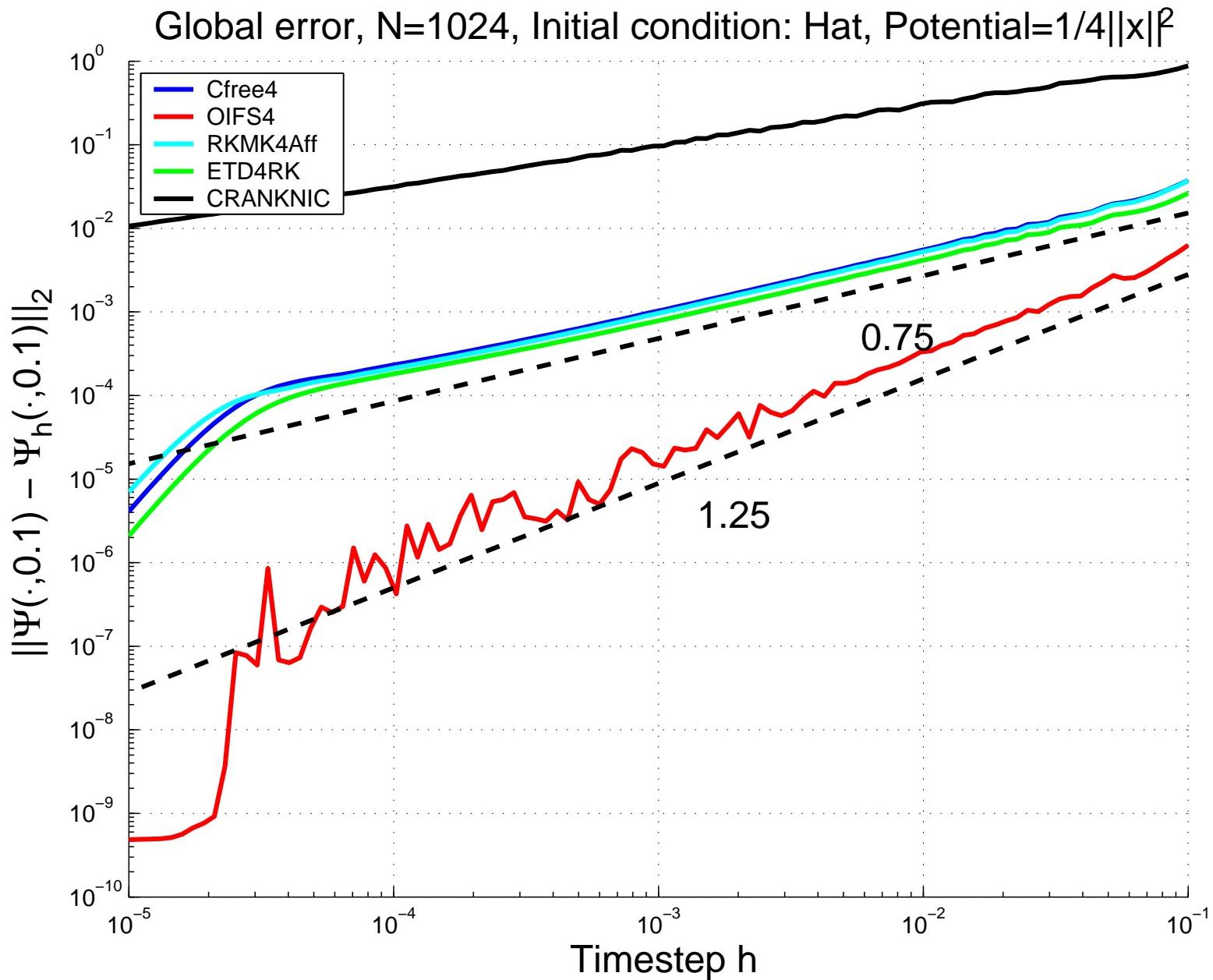


Figure 5

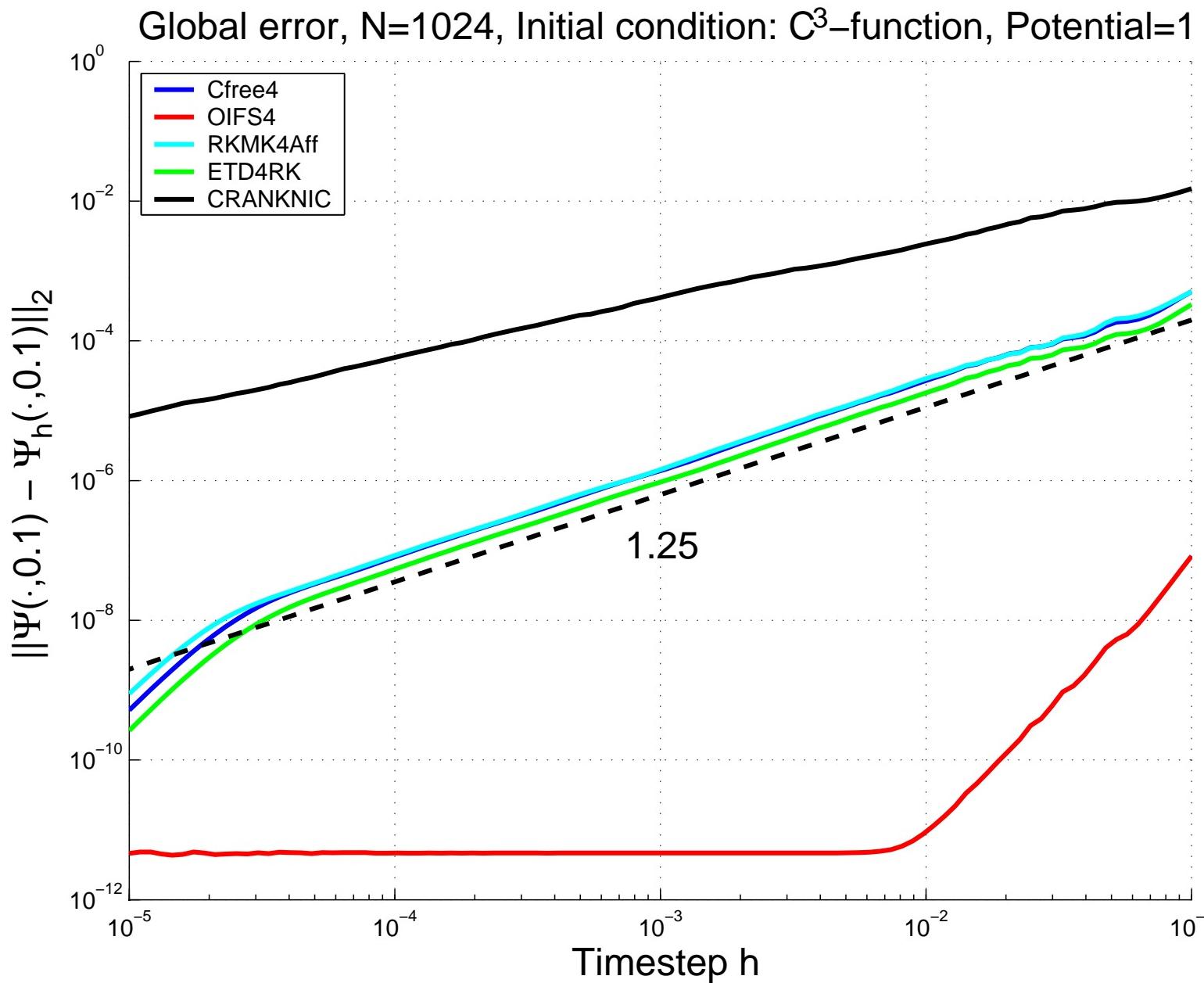


Figure 6

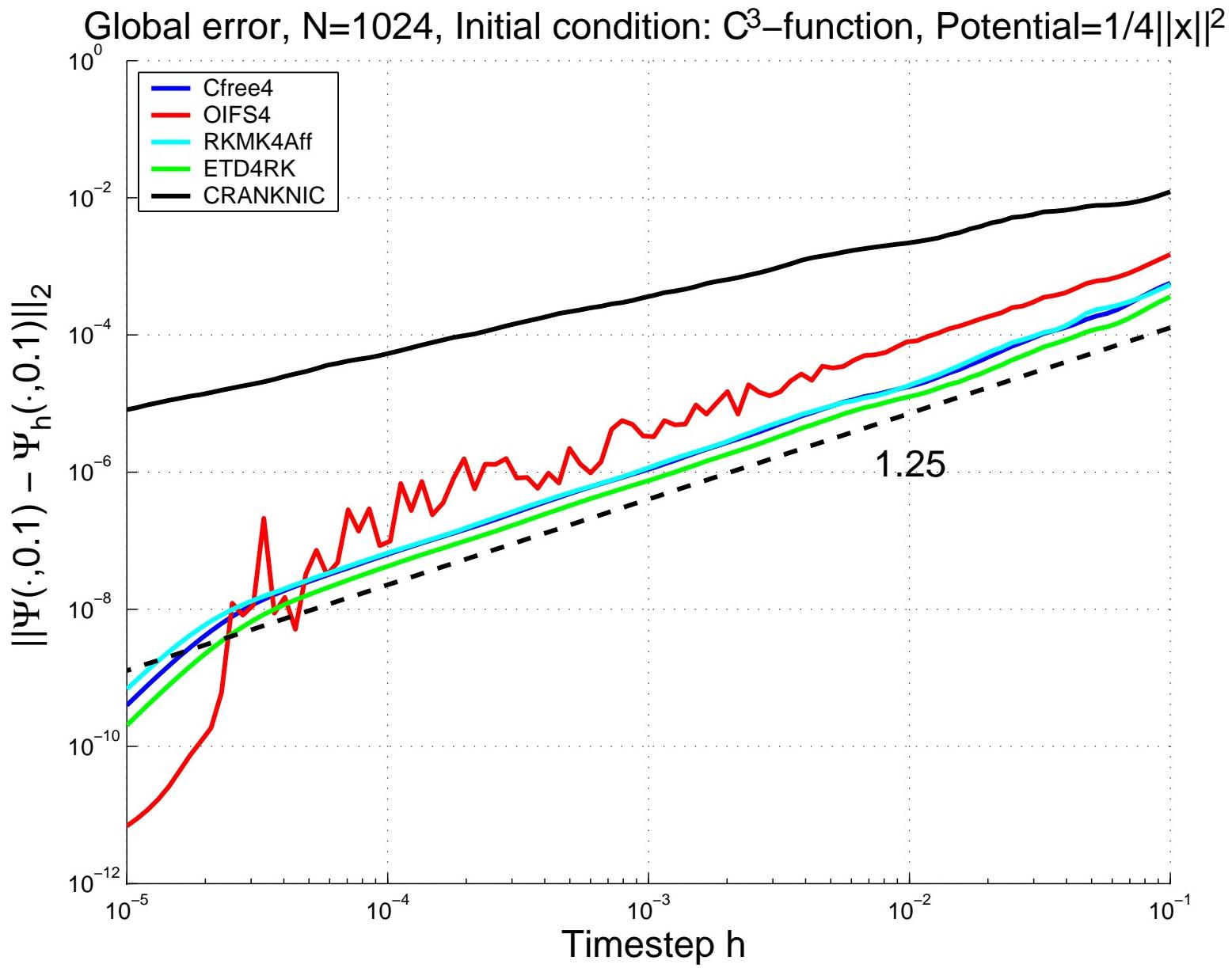


Figure 7

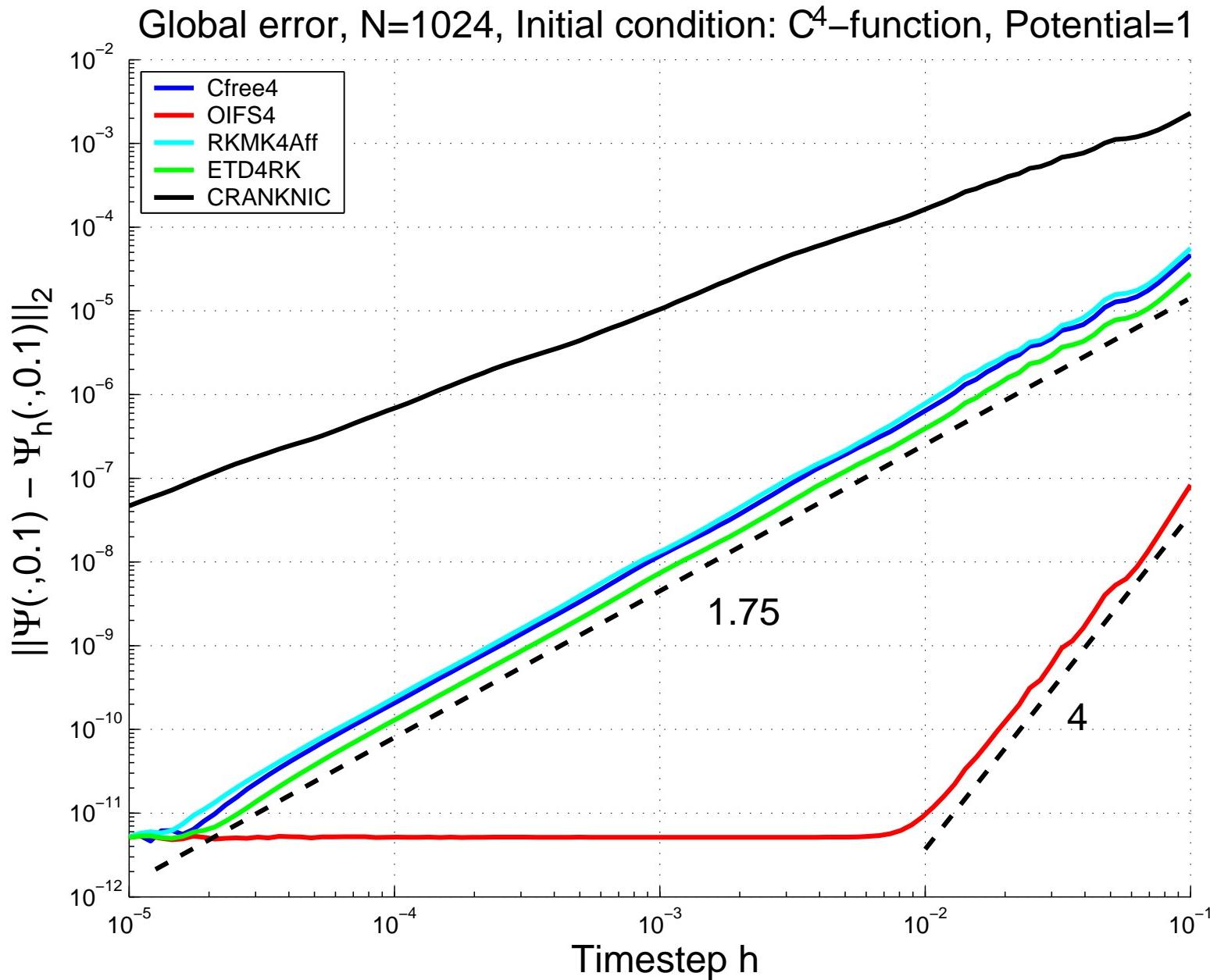


Figure 8

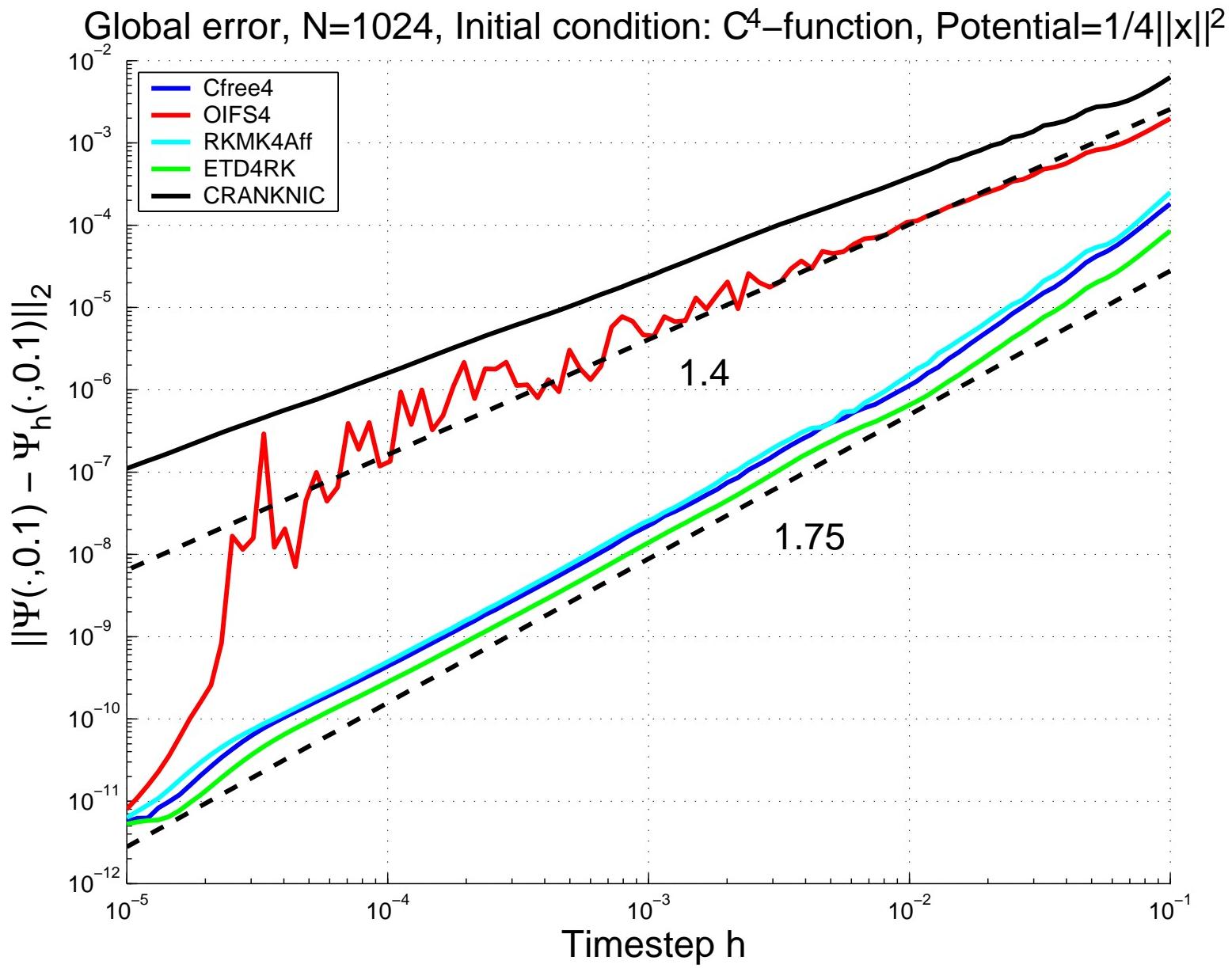


Figure 9

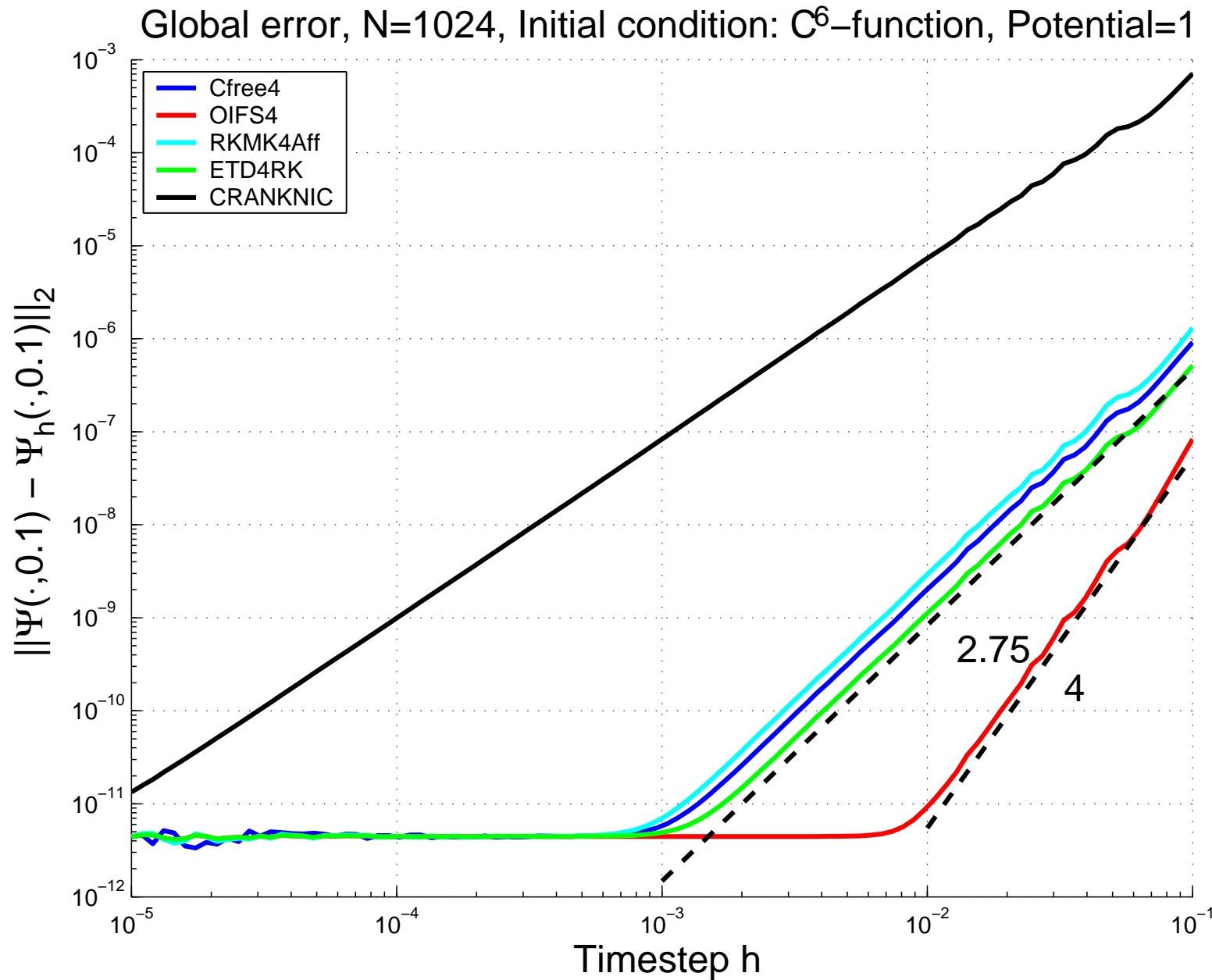
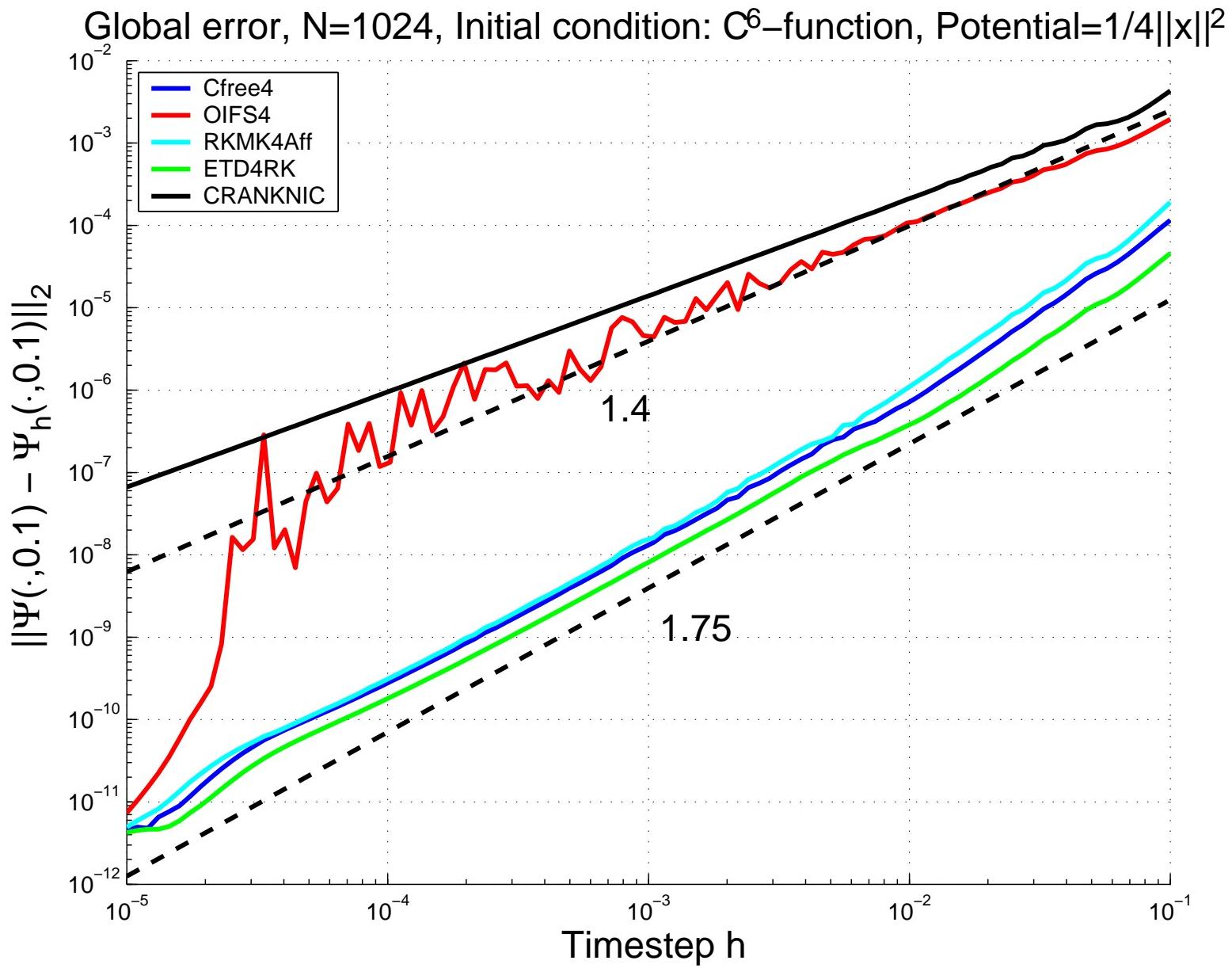


Figure 10



Our Work Plan

- Do this analysis for the other schemes
- Extend to more general $V(x)$
- Can the analysis include the nonlinear term?
Numerical tests show that it has little impact.
- We want to do the semiclassical case
- More space dimensions, more general boundary conditions
- Compare results with those from geometric integrators



Long Time Integration

For systems with a symplectic structure, experience shows that retention of such a structure in the numerical scheme enhances the long time quality of integration. Consider ([Islas et al](#)) the following 1D nonlinear Schrödinger equation

$$iu_t = -u_{xx} - 2|u|^2 u$$

on the circle. It is a completely integrable Hamiltonian system in the variables (q, q^*) with

$$H(q, q^*) = i \int_0^L (|q|^4 - |q_x|^2) dx$$
$$\omega = \int_0^L (dq^* \wedge dq) dx$$



Possible Strategies

1. Find a **multisymplectic structure** **Reich (2000)** and discretise simultaneously in space and time to preserve this structure.
2. Introduce an integrable space discretization (**Ablowitz/Ladik**), the resulting ODE system is not canonical. So standard symplectic integrators cannot be used, one may then
 - (a) Use a Lie–Poisson type integrator based on the generating function technique
 - (b) Apply (locally) the Darboux transformation to obtain a standard canonical Hamiltonian system to which a symplectic scheme can be applied



A Multisymplectic Structure

The above Schrödinger equation can be written in the form

$$\mathbf{M}z_t + \mathbf{K}z_x = \nabla_z S(z), \quad z \in \mathbb{R}^4.$$

Here \mathbf{M} and \mathbf{K} are skew-symmetric 4×4 -matrices, and $S : \mathbb{R}^4 \rightarrow \mathbb{R}$.

The two matrices define symplectic structures ω, κ on $\mathbb{R}^{\text{rank}(\mathbf{M})}$ and $\mathbb{R}^{\text{rank}(\mathbf{K})}$.

$$\omega(U, V) = V^T \mathbf{M} U, \quad \kappa(U, V) = V^T \mathbf{K} U.$$

In NLS we let $a = \text{Re } u$, $b = \text{Im } u$, $z = (a, b, a_x, b_x)^T$ so

$$S(z) = \frac{1}{2}(a_x^2 + b_x^2 + (a^2 + b^2)^2).$$



Multisymplectic Cont'd

Let \mathbf{U}, \mathbf{V} be two solutions of the variational equation

$$\mathbf{M} dz_t + \mathbf{K} dz_x = \mathbf{D}_{zz} S(z) dz$$

It easily follows that this pair of solutions satisfies

$$\partial_t \omega(\mathbf{U}, \mathbf{V}) + \partial_x \kappa(\mathbf{U}, \mathbf{V}) = 0$$

the symplectic conservation law.

The simplest multisymplectic scheme is obtained as the concatenated midpoint rule:

$$\mathbf{M} \left(\frac{z_{i+\frac{1}{2}}^{j+1} - z_{i+\frac{1}{2}}^j}{\Delta t} \right) + \mathbf{K} \left(\frac{z_{i+1}^{j+\frac{1}{2}} - z_i^{j+\frac{1}{2}}}{\Delta x} \right) = \nabla_z S \left(z_{i+\frac{1}{2}}^{j+\frac{1}{2}} \right)$$

The Ablowitz–Ladik Truncation

For simplicity, set $\mathbf{q} = \mathbf{u}$ and $\mathbf{p} = \mathbf{u}^*$. The above NLS now has the formulation

$$\begin{aligned} iq_t &= -q_{xx} - 2q^2 p \\ -ip_t &= -p_{xx} - 2p^2 q \end{aligned}$$

Semidiscretised version

$$\begin{aligned} i\dot{q}_n &= -\frac{q_{n-1} + q_{n+1} - 2q_n}{(\Delta x)^2} - p_n q_n (q_{n-1} + q_{n+1}) \\ -i\dot{p}_n &= -\frac{p_{n-1} + p_{n+1} - 2p_n}{(\Delta x)^2} - p_n q_n (p_{n-1} + p_{n+1}) \end{aligned}$$

AL Truncation Cont'd

It has a noncanonical Hamiltonian form

$$\dot{z} = P(z) \nabla H(z), \quad z = (p, q)$$

$$H = \frac{i}{(\Delta x)^3} \sum_n (\Delta x)^2 p_n (q_{n-1} + q_{n+1}) -$$

$$2 \ln(1 + (\Delta x)^2 q_n p_n)$$

$$P(z) = \begin{pmatrix} 0 & -R \\ R & 0 \end{pmatrix}$$

$$R = \text{diag} \left\{ \frac{1 + (\Delta x)^2 q_n p_n}{\Delta x} \right\}_{n=1}^N$$



Conclusions—Structure Preserving Integrators

- The literature ([Islas et al.](#)) report excellent long time behaviour of the presented approaches.
- Which approach is best depends on the parameters of the problems and the properties of interest.
- It is admitted that these geometric integrators are more expensive than classical ones.

